

# 2-Cyano-2-nitroadamantane

<b>Inchi:</b>	InChI=1S/C11H14N2O2/c12-6-11(13(14)15)9-2-7-1-8(4-9)5-10(11)3-7/h7-10H,1-5H2
<b>InchiKey:</b>	XQLWYBZMHPYUES-UHFFFAOYSA-N
<b>Formula:</b>	C11H14N2O2
<b>SMILES:</b>	N#CC1([N+](=O)[O-])C2CC3CC(C2)CC1C3
<b>Mol. weight [g/mol]:</b>	206.24
<b>CAS:</b>	128478-71-7

## Physical Properties

Property code	Value	Unit	Source
chs	-6238.40 ± 1.60	kJ/mol	NIST Webbook
gf	359.71	kJ/mol	Joback Method
hf	-21.00 ± 2.50	kJ/mol	NIST Webbook
hfs	-91.00 ± 1.60	kJ/mol	NIST Webbook
hfus	25.26	kJ/mol	Joback Method
hsub	70.00 ± 1.90	kJ/mol	NIST Webbook
hvap	65.29	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.982		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	720.39	K	Joback Method
tc	980.26	K	Joback Method
tf	488.05	K	Joback Method
vc	0.619	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.75	J/mol×K	720.39	Joback Method
cpg	488.63	J/mol×K	763.70	Joback Method
cpg	503.81	J/mol×K	807.01	Joback Method
cpg	518.60	J/mol×K	850.33	Joback Method
cpg	533.33	J/mol×K	893.64	Joback Method
cpg	548.30	J/mol×K	936.95	Joback Method

cpg	563.83	J/mol×K	980.26	Joback Method
hfust	4.98	kJ/mol	470.20	NIST Webbook
hsubt	70.00 ± 1.90	kJ/mol	337.50	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C128478717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128478717&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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